



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:33 pm BST

PDB ID : 3VMA  
Title : Crystal Structure of the Full-Length Transglycosylase PBP1b from Escherichia coli  
Authors : Huang, C.Y.; Sung, M.T.; Lai, Y.T.; Chou, L.Y.; Shih, H.W.; Cheng, W.C.; Wong, C.H.; Ma, C.  
Deposited on : 2011-12-09  
Resolution : 2.16 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

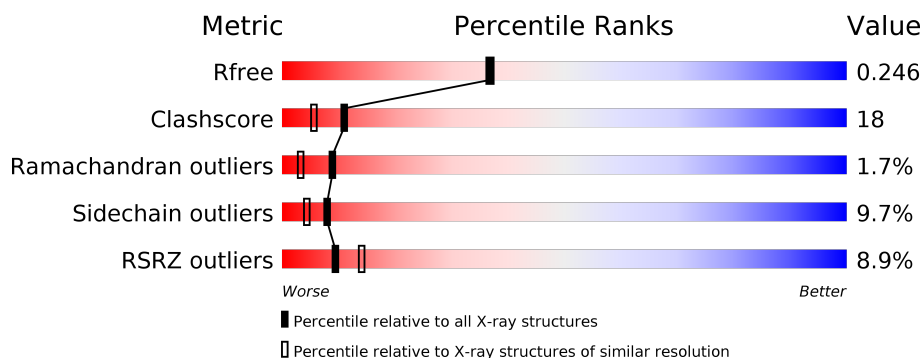
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	768	<div> <div>8%</div> <div> <div></div> <div>63%</div> <div>24%</div> <div>5%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5855 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

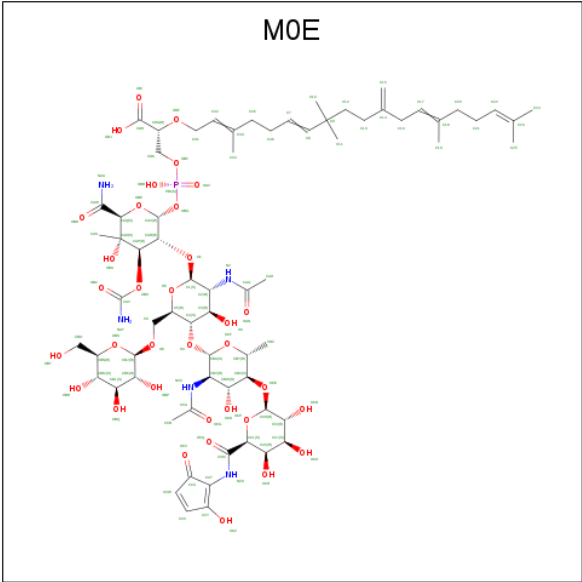
- Molecule 1 is a protein called Penicillin-binding protein 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	0	0
			5561	3524	981	1030	26			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	EXPRESSION TAG	UNP P02919
A	38	GLY	-	EXPRESSION TAG	UNP P02919
A	39	SER	-	EXPRESSION TAG	UNP P02919
A	40	SER	-	EXPRESSION TAG	UNP P02919
A	41	HIS	-	EXPRESSION TAG	UNP P02919
A	42	HIS	-	EXPRESSION TAG	UNP P02919
A	43	HIS	-	EXPRESSION TAG	UNP P02919
A	44	HIS	-	EXPRESSION TAG	UNP P02919
A	45	HIS	-	EXPRESSION TAG	UNP P02919
A	46	HIS	-	EXPRESSION TAG	UNP P02919
A	47	SER	-	EXPRESSION TAG	UNP P02919
A	48	SER	-	EXPRESSION TAG	UNP P02919
A	49	GLY	-	EXPRESSION TAG	UNP P02919
A	50	LEU	-	EXPRESSION TAG	UNP P02919
A	51	VAL	-	EXPRESSION TAG	UNP P02919
A	52	PRO	-	EXPRESSION TAG	UNP P02919
A	53	ARG	-	EXPRESSION TAG	UNP P02919
A	54	GLY	-	EXPRESSION TAG	UNP P02919
A	55	SER	-	EXPRESSION TAG	UNP P02919
A	56	HIS	-	EXPRESSION TAG	UNP P02919
A	57	MET	-	EXPRESSION TAG	UNP P02919

- Molecule 2 is MOENOMYCIN (three-letter code: M0E) (formula:  $C_{69}H_{106}N_5O_{34}P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	77	39	5	32	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	217	Total	O	0	0
			217	217		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Chain A:

8%

63%

24%

5%

8%

Sequence: MET GLY SER SER HIS HIS HIS HIS SER SER GLY VAL PRO ARG GLY SER HIS LYS PRD ARG GLY LYS ARG GLY TRP LEU TRP LEU LEU LEU LYS L72 A73 L74 V75 F76 A77 V78 L79 A81 L82 L85 V86 A90 I91 L102 P103 M110 V111 F112 L113

Sequence: E239 E240 ASP GLY ILE SER LEU Y246 S247 I248 G249 R250 A251 VAL LEU VAL ALA ASN V147 Q148 THR A155 S164 R170 L173 T174 A175 L180 F195 Q270 L196 L197 D198 P199 L276 L277 L278 S279 S280 E281 R282 Y284 L285 R286 N289 E290 A291 L295 L296 V297 S302 K303 R304 R305 L307 Y310 M311 Y315 Q318 D321 F327 P328 L329 Y334 F335 E340 D344 Q346 Q347 L350 V351 A352 M353 V354 K355 G356 A357 S358 I359 N360 P361 W362 R363 R364 K367 L368 A369 L370 E371 R372 L375 V376 L377 R378 L379 L380 Q381 Q382 Q383 Q384 I385 L393 G394 P395 N400 R401 R403 R404 G405 G406 V407 I408 S409 P410 L422 D428 K429 V430 K431 D432 I438 E451 V455 I458 P459 R465 K466 L467 L470 R465 A486 N487 L494 Q494 F499 N499 R506 S507 L511 L512 A520

Sequence: T670 L671 W672 T673 W674 W675 W676 W677 Q685 P689 L693 H694 L695 D707 T708 W709 Y734 S741 Q744 R745 Y746 Q750 L757 E761 D762 M766 N773 F774 W775 C776 W785 W786 T787 S788 D789 F790 Q791 S792 L793 C794 Q795 Q796 S797 E798 W799 D800 G1N

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.90Å 289.53Å 62.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.84 – 2.16 28.84 – 2.16	Depositor EDS
% Data completeness (in resolution range)	97.0 (28.84-2.16) 97.0 (28.84-2.16)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.212 , 0.250 0.208 , 0.246	Depositor DCC
$R_{free}$ test set	3072 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.063 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5855	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M0E

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/5672	0.49	0/7694

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5561	0	5598	202	0
2	A	77	0	60	7	0
3	A	217	0	0	4	0
All	All	5855	0	5658	204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (204) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:HD11	1:A:290:GLU:HB3	1.41	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:GLN:HE21	1:A:791:GLN:N	1.61	0.96
1:A:380:LEU:HD13	1:A:386:ILE:HG13	1.49	0.95
1:A:787:THR:HG22	1:A:789:ASP:H	1.39	0.88
1:A:110:MET:HG2	1:A:199:PRO:HG3	1.53	0.88
1:A:671:LEU:HD13	1:A:674:MET:HE3	1.56	0.88
1:A:674:MET:HA	1:A:677:VAL:HG13	1.59	0.83
1:A:665:GLN:H	1:A:665:GLN:HE21	1.25	0.82
1:A:235:ARG:HD2	1:A:235:ARG:H	1.47	0.79
1:A:791:GLN:HE21	1:A:791:GLN:CA	1.97	0.77
1:A:110:MET:CG	1:A:199:PRO:HG3	2.14	0.76
1:A:303:LYS:HG3	1:A:304:ASP:H	1.51	0.75
1:A:665:GLN:H	1:A:665:GLN:NE2	1.84	0.75
1:A:307:LEU:O	1:A:311:MET:HG3	1.87	0.74
1:A:789:ASP:O	1:A:791:GLN:N	2.20	0.73
1:A:386:ILE:HG23	1:A:390:LEU:HD11	1.71	0.73
1:A:671:LEU:CD1	1:A:674:MET:HE3	2.21	0.70
1:A:674:MET:SD	3:A:1172:HOH:O	2.49	0.70
1:A:270:GLN:HE22	1:A:291:ALA:HA	1.56	0.70
1:A:355:LYS:HG2	2:A:901:M0E:HAS1	1.73	0.70
1:A:401:VAL:HG12	1:A:402:GLN:H	1.58	0.69
1:A:790:PRO:O	1:A:793:LEU:HG	1.92	0.69
1:A:384:GLN:HE21	1:A:384:GLN:H	1.41	0.69
1:A:359:ILE:HD12	2:A:901:M0E:HCB1	1.73	0.69
1:A:375:LEU:O	1:A:378:ARG:HG3	1.93	0.69
1:A:380:LEU:HD13	1:A:386:ILE:CG1	2.23	0.67
1:A:670:THR:HG22	1:A:674:MET:HE1	1.75	0.67
1:A:384:GLN:NE2	1:A:384:GLN:H	1.93	0.66
1:A:741:SER:O	1:A:744:GLN:HG2	1.96	0.66
1:A:670:THR:HG22	1:A:674:MET:CE	2.26	0.65
1:A:506:ARG:HD2	1:A:707:ASP:OD1	1.94	0.65
1:A:766:MET:HE3	1:A:793:LEU:HD23	1.77	0.65
1:A:238:TYR:O	1:A:240:HIS:N	2.30	0.64
1:A:359:ILE:H	1:A:359:ILE:HD13	1.62	0.64
1:A:385:ILE:H	1:A:385:ILE:HD13	1.63	0.64
1:A:381:GLN:HA	1:A:386:ILE:HB	1.78	0.64
1:A:72:LEU:HD23	1:A:74:ILE:HB	1.79	0.64
1:A:222:PRO:HD2	1:A:225:LEU:HD22	1.80	0.63
1:A:791:GLN:HG3	1:A:794:CYS:SG	2.39	0.63
1:A:234:ASP:OD1	1:A:268:LEU:HB2	1.99	0.63
1:A:363:TRP:HH2	1:A:403:PRO:HB2	1.64	0.62
1:A:628:ILE:HD11	1:A:671:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:PRO:C	1:A:791:GLN:HE21	2.02	0.62
1:A:173:LEU:N	1:A:173:LEU:HD12	2.15	0.61
1:A:593:TRP:O	1:A:598:VAL:HG22	2.00	0.60
1:A:387:ASP:HB2	1:A:390:LEU:HG	1.83	0.60
1:A:344:LEU:HD21	1:A:386:ILE:HD11	1.84	0.60
1:A:407:VAL:HG13	1:A:410:PRO:HG3	1.84	0.60
1:A:363:TRP:HZ3	1:A:404:ARG:HA	1.67	0.59
1:A:221:PHE:HB3	1:A:225:LEU:HD21	1.84	0.59
1:A:694:HIS:HD2	3:A:1146:HOH:O	1.86	0.59
1:A:377:LEU:HA	1:A:380:LEU:HD11	1.84	0.59
1:A:222:PRO:HG3	1:A:340:GLU:HA	1.84	0.58
1:A:670:THR:O	1:A:674:MET:HE2	2.03	0.58
1:A:75:VAL:O	1:A:79:LEU:HD13	2.02	0.58
1:A:785:VAL:HG12	1:A:787:THR:OG1	2.03	0.58
1:A:303:LYS:HG3	1:A:304:ASP:N	2.18	0.58
1:A:206:SER:HA	1:A:212:GLN:HE22	1.68	0.58
1:A:526:ILE:HG13	1:A:527:TYR:CD2	2.39	0.58
1:A:402:GLN:O	1:A:404:ARG:HG3	2.02	0.58
1:A:139:MET:HG3	1:A:146:THR:HG23	1.86	0.57
1:A:795:GLN:O	1:A:798:GLU:HG2	2.03	0.57
1:A:356:GLY:O	1:A:360:TYR:HD2	1.88	0.57
1:A:79:LEU:HA	1:A:82:ILE:HG12	1.86	0.57
1:A:693:LEU:HB3	1:A:695:LEU:HD13	1.86	0.56
1:A:799:MET:HG3	1:A:800:GLN:H	1.70	0.56
1:A:175:PHE:HB3	3:A:1161:HOH:O	2.05	0.56
1:A:304:ASP:HA	1:A:307:LEU:HD21	1.87	0.56
1:A:789:ASP:C	1:A:791:GLN:H	2.08	0.56
1:A:363:TRP:HZ3	1:A:404:ARG:CA	2.19	0.55
1:A:422:LEU:HD11	1:A:438:ILE:HD13	1.88	0.55
1:A:530:ASN:HD22	1:A:530:ASN:H	1.54	0.55
1:A:791:GLN:NE2	1:A:791:GLN:CA	2.69	0.55
1:A:685:GLN:HE21	1:A:689:LYS:NZ	2.04	0.55
1:A:276:LEU:HD22	1:A:277:PHE:CZ	2.42	0.54
1:A:351:VAL:O	1:A:354:VAL:HG12	2.06	0.54
1:A:401:VAL:HG12	1:A:402:GLN:N	2.22	0.53
1:A:350:LEU:HA	1:A:353:MET:HE2	1.91	0.53
1:A:75:VAL:O	1:A:78:VAL:HB	2.09	0.53
1:A:283:SER:HB3	1:A:286:ARG:H	1.74	0.53
1:A:542:GLN:HB2	1:A:543:PRO:HD2	1.90	0.53
1:A:267:THR:O	1:A:271:GLN:HG3	2.09	0.52
1:A:799:MET:HG3	1:A:800:GLN:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:MET:CE	1:A:793:LEU:HD23	2.38	0.52
1:A:402:GLN:NE2	1:A:403:PRO:HD2	2.25	0.52
1:A:356:GLY:HA3	1:A:359:ILE:HD11	1.91	0.52
1:A:361:ASN:HD21	1:A:363:TRP:HD1	1.58	0.52
1:A:278:LEU:CD1	1:A:290:GLU:HB3	2.28	0.52
1:A:334:TYR:O	1:A:335:PHE:CG	2.63	0.52
1:A:741:SER:HA	1:A:744:GLN:CD	2.30	0.51
2:A:901:M0E:ODI	2:A:901:M0E:HAQ	2.11	0.51
1:A:307:LEU:HA	1:A:310:TYR:HB3	1.91	0.51
1:A:235:ARG:HD2	1:A:235:ARG:N	2.22	0.51
1:A:377:LEU:O	1:A:381:GLN:HB3	2.10	0.51
1:A:403:PRO:O	1:A:404:ARG:HD3	2.10	0.51
1:A:376:VAL:O	1:A:380:LEU:HG	2.11	0.51
1:A:364:ARG:N	1:A:364:ARG:HD2	2.26	0.51
1:A:372:ARG:O	1:A:376:VAL:HG23	2.11	0.51
1:A:250:ARG:O	1:A:250:ARG:HD2	2.10	0.51
1:A:307:LEU:H	1:A:307:LEU:HD23	1.74	0.51
1:A:315:TYR:OH	1:A:318:GLN:HB2	2.10	0.51
1:A:431:LYS:HE2	1:A:431:LYS:H	1.76	0.51
1:A:776:CYS:HA	1:A:793:LEU:HD13	1.93	0.51
1:A:591:GLU:HG2	1:A:595:LYS:HE3	1.93	0.50
1:A:246:TYR:HE1	1:A:250:ARG:HB2	1.77	0.50
1:A:173:LEU:CD1	1:A:173:LEU:N	2.74	0.50
1:A:286:ARG:O	1:A:290:GLU:HG2	2.12	0.50
1:A:355:LYS:O	2:A:901:M0E:H5	2.11	0.50
1:A:520:ALA:HB2	1:A:584:LEU:HD11	1.92	0.49
1:A:674:MET:HA	1:A:677:VAL:CG1	2.37	0.49
1:A:131:THR:HG22	1:A:131:THR:O	2.12	0.49
1:A:327:PHE:N	1:A:328:PRO:CD	2.75	0.49
1:A:536:ALA:HB1	1:A:537:PRO:HD2	1.93	0.49
1:A:633:ASN:HD22	1:A:660:ARG:HA	1.77	0.49
1:A:776:CYS:SG	1:A:793:LEU:HD13	2.53	0.49
1:A:428:ASP:O	1:A:431:LYS:HE3	2.12	0.49
1:A:72:LEU:HD23	1:A:74:ILE:H	1.77	0.49
1:A:76:PHE:O	1:A:80:ILE:HG23	2.13	0.48
1:A:552:ASN:ND2	1:A:575:VAL:H	2.11	0.48
1:A:403:PRO:O	1:A:405:GLY:N	2.46	0.48
2:A:901:M0E:H61	2:A:901:M0E:CCA	2.44	0.48
1:A:385:ILE:HG12	1:A:386:ILE:HG12	1.95	0.48
1:A:392:ASP:OD1	1:A:393:MET:N	2.46	0.48
1:A:670:THR:C	1:A:674:MET:HE2	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:LEU:HB3	1:A:757:LEU:HD11	1.96	0.47
1:A:470:LEU:N	3:A:1170:HOH:O	2.48	0.47
1:A:344:LEU:HD23	1:A:394:LEU:HD11	1.97	0.46
1:A:774:PHE:N	1:A:796:GLN:HG2	2.30	0.46
1:A:487:MET:HE1	1:A:619:ILE:HD12	1.98	0.46
1:A:72:LEU:CD2	1:A:74:ILE:HB	2.45	0.46
1:A:302:SER:O	1:A:306:ILE:HG12	2.15	0.46
1:A:380:LEU:HD12	1:A:381:GLN:N	2.30	0.46
1:A:91:ILE:HG22	1:A:91:ILE:O	2.16	0.46
1:A:340:GLU:O	1:A:340:GLU:HG2	2.15	0.46
1:A:237:PHE:O	1:A:238:TYR:HB3	2.16	0.46
1:A:375:LEU:HD23	1:A:379:LEU:HG	1.97	0.46
1:A:451:GLU:O	1:A:455:VAL:HG23	2.16	0.45
1:A:407:VAL:HG12	1:A:407:VAL:O	2.15	0.45
1:A:467:LEU:HD12	1:A:470:LEU:HD22	1.98	0.45
1:A:511:LEU:HD22	1:A:709:TRP:CB	2.47	0.45
1:A:350:LEU:HA	1:A:353:MET:CE	2.46	0.45
1:A:315:TYR:HD1	1:A:357:ALA:CB	2.30	0.45
1:A:344:LEU:HD21	1:A:386:ILE:CD1	2.47	0.45
1:A:135:GLN:HB2	1:A:145:PHE:CZ	2.52	0.45
1:A:665:GLN:O	1:A:669:LEU:HG	2.16	0.45
1:A:685:GLN:NE2	1:A:689:LYS:NZ	2.65	0.45
1:A:344:LEU:HA	1:A:347:GLN:OE1	2.17	0.44
1:A:76:PHE:HA	1:A:79:LEU:CD1	2.47	0.44
1:A:530:ASN:N	1:A:530:ASN:HD22	2.09	0.44
1:A:685:GLN:HE21	1:A:689:LYS:HZ2	1.65	0.44
1:A:304:ASP:HA	1:A:307:LEU:CD2	2.46	0.44
1:A:359:ILE:CD1	1:A:359:ILE:H	2.30	0.44
1:A:553:ASP:OD1	1:A:553:ASP:C	2.56	0.44
1:A:586:LEU:N	1:A:587:PRO:CD	2.80	0.44
1:A:276:LEU:HD23	1:A:276:LEU:O	2.18	0.44
1:A:248:ILE:HD13	1:A:248:ILE:O	2.17	0.43
1:A:458:ILE:HB	1:A:459:PRO:HD3	2.00	0.43
1:A:221:PHE:HB3	1:A:225:LEU:CD2	2.47	0.43
1:A:393:MET:HE2	1:A:393:MET:O	2.18	0.43
1:A:383:GLN:HB2	1:A:385:ILE:CD1	2.49	0.43
1:A:79:LEU:HD13	1:A:79:LEU:H	1.83	0.43
1:A:238:TYR:N	1:A:238:TYR:CD2	2.87	0.43
1:A:390:LEU:HD12	1:A:391:TYR:N	2.33	0.43
1:A:507:SER:HA	1:A:615:ASN:HD22	1.83	0.43
1:A:673:THR:O	1:A:676:GLN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PHE:HA	1:A:79:LEU:HD11	1.99	0.43
1:A:789:ASP:OD2	1:A:791:GLN:HB2	2.18	0.43
1:A:113:LEU:HD12	1:A:195:PHE:HD1	1.83	0.43
1:A:218:ARG:HG3	1:A:304:ASP:HB3	2.01	0.43
1:A:761:GLU:O	1:A:762:ASP:HB2	2.18	0.43
1:A:115:PRO:O	1:A:116:ASP:HB2	2.19	0.42
1:A:575:VAL:HB	1:A:576:PRO:HD3	2.01	0.42
1:A:315:TYR:HD1	1:A:357:ALA:HB1	1.85	0.42
1:A:403:PRO:C	1:A:404:ARG:HD3	2.40	0.42
1:A:487:MET:CE	1:A:619:ILE:HD12	2.49	0.42
1:A:544:ASN:N	1:A:544:ASN:HD22	2.17	0.42
1:A:225:LEU:HD23	1:A:226:VAL:N	2.33	0.42
1:A:355:LYS:O	2:A:901:M0E:H1	2.20	0.42
1:A:285:TRP:O	1:A:289:ASN:HB2	2.20	0.42
1:A:746:TYR:CE2	1:A:750:GLN:NE2	2.87	0.42
1:A:335:PHE:CE1	1:A:346:GLN:HG2	2.54	0.41
1:A:791:GLN:NE2	1:A:791:GLN:N	2.46	0.41
1:A:102:LEU:HA	1:A:103:PRO:HD2	1.90	0.41
1:A:234:ASP:CG	1:A:238:TYR:HB3	2.41	0.41
1:A:271:GLN:OE1	2:A:901:M0E:HAH2	2.20	0.41
1:A:205:ILE:O	1:A:206:SER:C	2.59	0.41
1:A:741:SER:HA	1:A:744:GLN:OE1	2.20	0.41
1:A:250:ARG:O	1:A:251:ALA:HB2	2.21	0.41
1:A:773:ASN:HB3	1:A:796:GLN:CG	2.50	0.41
1:A:399:LEU:HD22	1:A:399:LEU:N	2.36	0.41
1:A:155:ILE:HG12	1:A:170:ARG:HG3	2.02	0.41
1:A:232:THR:O	1:A:233:GLU:C	2.59	0.41
1:A:544:ASN:HA	1:A:545:GLY:HA2	1.42	0.41
1:A:356:GLY:O	1:A:360:TYR:CD2	2.72	0.41
1:A:378:ARG:HD2	1:A:378:ARG:C	2.41	0.41
1:A:385:ILE:O	1:A:386:ILE:HD13	2.20	0.41
1:A:392:ASP:OD1	1:A:392:ASP:C	2.59	0.41
1:A:604:HIS:HA	1:A:605:PRO:HD3	1.94	0.41
1:A:133:TYR:CE1	1:A:143:GLY:HA2	2.56	0.41
1:A:238:TYR:C	1:A:238:TYR:CD2	2.91	0.41
1:A:406:GLY:O	1:A:407:VAL:C	2.59	0.40
1:A:499:ASN:ND2	1:A:499:ASN:C	2.74	0.40
1:A:334:TYR:O	1:A:403:PRO:HD3	2.21	0.40
1:A:552:ASN:HD21	1:A:575:VAL:H	1.68	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	700/768 (91%)	645 (92%)	43 (6%)	12 (2%)	9 3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	TYR
1	A	239	GLU
1	A	404	ARG
1	A	790	PRO
1	A	233	GLU
1	A	283	SER
1	A	544	ASN
1	A	407	VAL
1	A	164	SER
1	A	206	SER
1	A	335	PHE
1	A	430	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	597/645 (93%)	539 (90%)	58 (10%)	8 4

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	79	LEU
1	A	86	TYR
1	A	112	ASN
1	A	148	GLN
1	A	173	LEU
1	A	180	LEU
1	A	197	LEU
1	A	212	GLN
1	A	218	ARG
1	A	225	LEU
1	A	226	VAL
1	A	233	GLU
1	A	234	ASP
1	A	235	ARG
1	A	236	HIS
1	A	237	PHE
1	A	238	TYR
1	A	246	TYR
1	A	247	SER
1	A	248	ILE
1	A	268	LEU
1	A	270	GLN
1	A	272	LEU
1	A	281	GLU
1	A	289	ASN
1	A	321	ASP
1	A	359	ILE
1	A	368	LEU
1	A	372	ARG
1	A	380	LEU
1	A	381	GLN
1	A	384	GLN
1	A	385	ILE
1	A	402	GLN
1	A	404	ARG
1	A	408	ILE
1	A	431	LYS
1	A	465	ARG
1	A	466	LYS
1	A	485	ARG
1	A	495	PHE
1	A	499	ASN

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Mol	Chain	Res	Type
1	A	530	ASN
1	A	544	ASN
1	A	546	GLN
1	A	555	ARG
1	A	559	GLU
1	A	572	SER
1	A	609	MET
1	A	628	ILE
1	A	641	ARG
1	A	665	GLN
1	A	671	LEU
1	A	685	GLN
1	A	695	LEU
1	A	750	GLN
1	A	791	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	112	ASN
1	A	179	HIS
1	A	191	GLN
1	A	212	GLN
1	A	240	HIS
1	A	270	GLN
1	A	275	ASN
1	A	289	ASN
1	A	318	GLN
1	A	381	GLN
1	A	383	GLN
1	A	384	GLN
1	A	388	GLN
1	A	402	GLN
1	A	411	GLN
1	A	423	GLN
1	A	499	ASN
1	A	503	GLN
1	A	523	GLN
1	A	530	ASN
1	A	544	ASN
1	A	552	ASN

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Mol	Chain	Res	Type
1	A	615	ASN
1	A	633	ASN
1	A	657	GLN
1	A	665	GLN
1	A	685	GLN
1	A	703	ASN
1	A	791	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	M0E	A	901	-	76,81,114	1.99	20 (26%)	110,122,166	2.63	52 (47%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M0E	A	901	-	-	11/47/158/206	0/5/5/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	M0E	CAV-NAT	5.85	1.44	1.33
2	A	901	M0E	C3-C2	5.45	1.63	1.53
2	A	901	M0E	C1-C2	5.02	1.61	1.53
2	A	901	M0E	CCM-NCS	4.38	1.44	1.32
2	A	901	M0E	CAW-NAU	4.32	1.43	1.32
2	A	901	M0E	OBH-CAV	-3.68	1.27	1.35
2	A	901	M0E	OBC-CAV	3.65	1.26	1.21
2	A	901	M0E	OBH-CAP	-3.23	1.39	1.45
2	A	901	M0E	CCA-NCC	3.11	1.45	1.34
2	A	901	M0E	CAG-N2	3.11	1.45	1.34
2	A	901	M0E	CAX-CAR	3.02	1.60	1.52
2	A	901	M0E	CAO-CAP	-2.89	1.49	1.54
2	A	901	M0E	OBA-CAO	-2.68	1.39	1.44
2	A	901	M0E	CBU-CBV	2.52	1.57	1.53
2	A	901	M0E	OBE-CAX	2.31	1.47	1.41
2	A	901	M0E	ODF-CDG	-2.07	1.38	1.42
2	A	901	M0E	CBX-CBY	2.04	1.56	1.52
2	A	901	M0E	OCN-CCI	-2.03	1.38	1.43
2	A	901	M0E	O3-C3	-2.02	1.38	1.43
2	A	901	M0E	CBW-CBV	2.00	1.57	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	M0E	CAS-CAO-CAQ	-10.32	102.79	111.11
2	A	901	M0E	O5-C5-C6	6.08	118.94	106.67
2	A	901	M0E	OBH-CAV-NAT	5.87	119.71	110.58
2	A	901	M0E	OBH-CAP-CAO	5.18	115.51	108.12
2	A	901	M0E	O1-C1-C2	4.94	116.76	108.24
2	A	901	M0E	O6-CBJ-CBK	4.90	115.96	108.30
2	A	901	M0E	OBS-CBN-CBO	4.48	117.57	106.44
2	A	901	M0E	OCF-CBY-CBZ	4.20	115.76	106.70
2	A	901	M0E	OBH-CAP-CAR	4.04	116.53	108.00
2	A	901	M0E	O6-C6-C5	3.89	116.25	109.05
2	A	901	M0E	O4-C4-C3	3.87	117.58	107.28
2	A	901	M0E	CAS-CAO-CAP	3.87	115.94	111.28
2	A	901	M0E	OBE-CAX-OBG	3.82	116.36	111.36
2	A	901	M0E	O1-CAR-CAP	3.76	116.53	106.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	M0E	OBf-CDK-CDG	3.69	118.58	107.94
2	A	901	M0E	C6-O6-CBJ	3.67	120.91	113.74
2	A	901	M0E	OBH-CAV-OBC	-3.63	120.02	123.69
2	A	901	M0E	O4-CBU-CBV	3.44	114.18	108.24
2	A	901	M0E	OBG-CAX-CAR	3.44	114.68	108.38
2	A	901	M0E	OBP-CBK-CBL	3.42	118.25	110.35
2	A	901	M0E	C1-O1-CAR	-3.27	109.88	117.96
2	A	901	M0E	OBP-CBK-CBJ	3.26	117.96	110.05
2	A	901	M0E	OBC-CAV-NAT	-3.20	120.23	125.51
2	A	901	M0E	O3-C3-C2	3.13	115.98	109.66
2	A	901	M0E	OBS-CBJ-O6	3.01	117.11	109.97
2	A	901	M0E	OBQ-CBL-CBM	3.00	117.28	110.35
2	A	901	M0E	OCP-CCL-CCM	2.92	116.72	107.08
2	A	901	M0E	OCO-CCJ-CCI	2.90	117.06	110.35
2	A	901	M0E	OBA-CAO-CAQ	-2.87	101.89	107.66
2	A	901	M0E	OCE-CBX-CBW	2.87	114.91	107.28
2	A	901	M0E	OBR-CBM-CBN	2.84	116.35	109.30
2	A	901	M0E	OBE-CAQ-CAW	2.80	116.70	109.39
2	A	901	M0E	OCE-CBX-CBY	2.80	114.07	106.79
2	A	901	M0E	OCR-CCK-CCL	2.79	116.01	109.74
2	A	901	M0E	OBR-CBM-CBL	2.79	116.81	110.35
2	A	901	M0E	OBQ-CBL-CBK	2.75	116.70	110.35
2	A	901	M0E	OCE-CCH-CCI	2.60	114.83	108.10
2	A	901	M0E	C1-C2-N2	2.51	115.33	111.00
2	A	901	M0E	OCR-CCK-CCJ	2.46	116.04	110.35
2	A	901	M0E	OCD-CBW-CBV	2.45	114.61	109.66
2	A	901	M0E	C3-C2-N2	2.44	115.23	110.62
2	A	901	M0E	OBA-CAO-CAS	2.44	112.83	107.74
2	A	901	M0E	CCK-CCL-CCM	2.43	116.11	111.30
2	A	901	M0E	C1-O5-C5	-2.33	109.11	113.69
2	A	901	M0E	CBU-CBV-NCC	2.30	114.96	111.00
2	A	901	M0E	OCO-CCJ-CCK	2.30	115.66	110.35
2	A	901	M0E	O4-C4-C5	2.27	115.67	109.45
2	A	901	M0E	C6-C5-C4	2.23	118.84	113.33
2	A	901	M0E	CCH-OCE-CBX	-2.19	112.55	117.96
2	A	901	M0E	CAH-CAG-N2	2.17	119.77	116.10
2	A	901	M0E	O3-C3-C4	2.14	115.62	109.94
2	A	901	M0E	CCB-CCA-NCC	2.02	119.53	116.10

There are no chirality outliers.

All (11) torsion outliers are listed below:

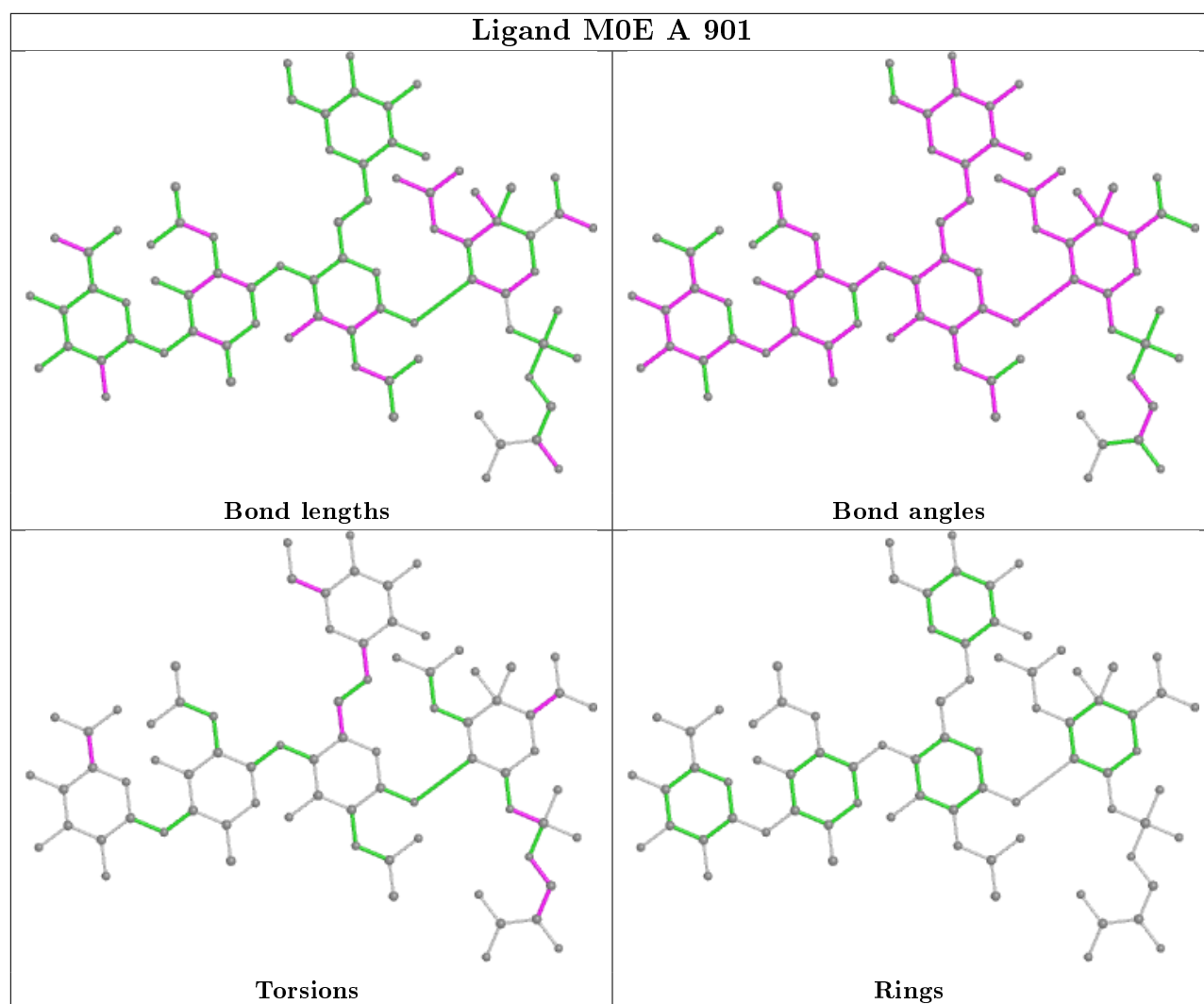
Mol	Chain	Res	Type	Atoms
2	A	901	M0E	ODF-CDG-CDK-OBF
2	A	901	M0E	CAX-OBG-PBI-OB
2	A	901	M0E	OBE-CAQ-CAW-NAU
2	A	901	M0E	OBS-CBJ-O6-C6
2	A	901	M0E	CCK-CCL-CCM-OCQ
2	A	901	M0E	CBM-CBN-CBO-OBT
2	A	901	M0E	C4-C5-C6-O6
2	A	901	M0E	CAX-OBG-PBI-OBF
2	A	901	M0E	CDG-CDK-OBF-PBI
2	A	901	M0E	CDH-CDG-CDK-OBF
2	A	901	M0E	OBE-CAQ-CAW-OB

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	M0E	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	708/768 (92%)	0.55	63 (8%) 9 14	32, 62, 152, 182	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	TRP	7.6
1	A	544	ASN	6.8
1	A	76	PHE	6.6
1	A	394	LEU	6.1
1	A	282	ARG	5.9
1	A	734	TYR	5.1
1	A	360	TYR	4.8
1	A	368	LEU	4.7
1	A	248	ILE	4.4
1	A	406	GLY	4.4
1	A	388	GLN	4.4
1	A	386	ILE	4.3
1	A	371	GLU	4.1
1	A	408	ILE	4.0
1	A	407	VAL	3.8
1	A	235	ARG	3.8
1	A	229	LEU	3.8
1	A	295	LEU	3.8
1	A	432	ASP	3.7
1	A	268	LEU	3.6
1	A	238	TYR	3.6
1	A	77	ALA	3.6
1	A	369	ALA	3.6
1	A	382	GLN	3.6
1	A	86	TYR	3.5
1	A	401	VAL	3.4
1	A	90	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	270	GLN	3.4
1	A	74	ILE	3.3
1	A	297	MET	3.2
1	A	234	ASP	3.1
1	A	379	LEU	3.0
1	A	231	ALA	3.0
1	A	357	ALA	3.0
1	A	78	VAL	2.9
1	A	390	LEU	2.9
1	A	75	VAL	2.9
1	A	378	ARG	2.9
1	A	399	LEU	2.9
1	A	85	VAL	2.8
1	A	494	GLN	2.8
1	A	307	LEU	2.8
1	A	246	TYR	2.8
1	A	367	LYS	2.8
1	A	280	SER	2.7
1	A	233	GLU	2.5
1	A	800	GLN	2.5
1	A	335	PHE	2.5
1	A	495	PHE	2.5
1	A	236	HIS	2.4
1	A	306	ILE	2.4
1	A	385	ILE	2.4
1	A	355	LYS	2.4
1	A	91	ILE	2.4
1	A	380	LEU	2.3
1	A	329	LEU	2.2
1	A	467	LEU	2.1
1	A	393	MET	2.1
1	A	466	LYS	2.1
1	A	364	ARG	2.1
1	A	79	LEU	2.1
1	A	389	GLU	2.1
1	A	375	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

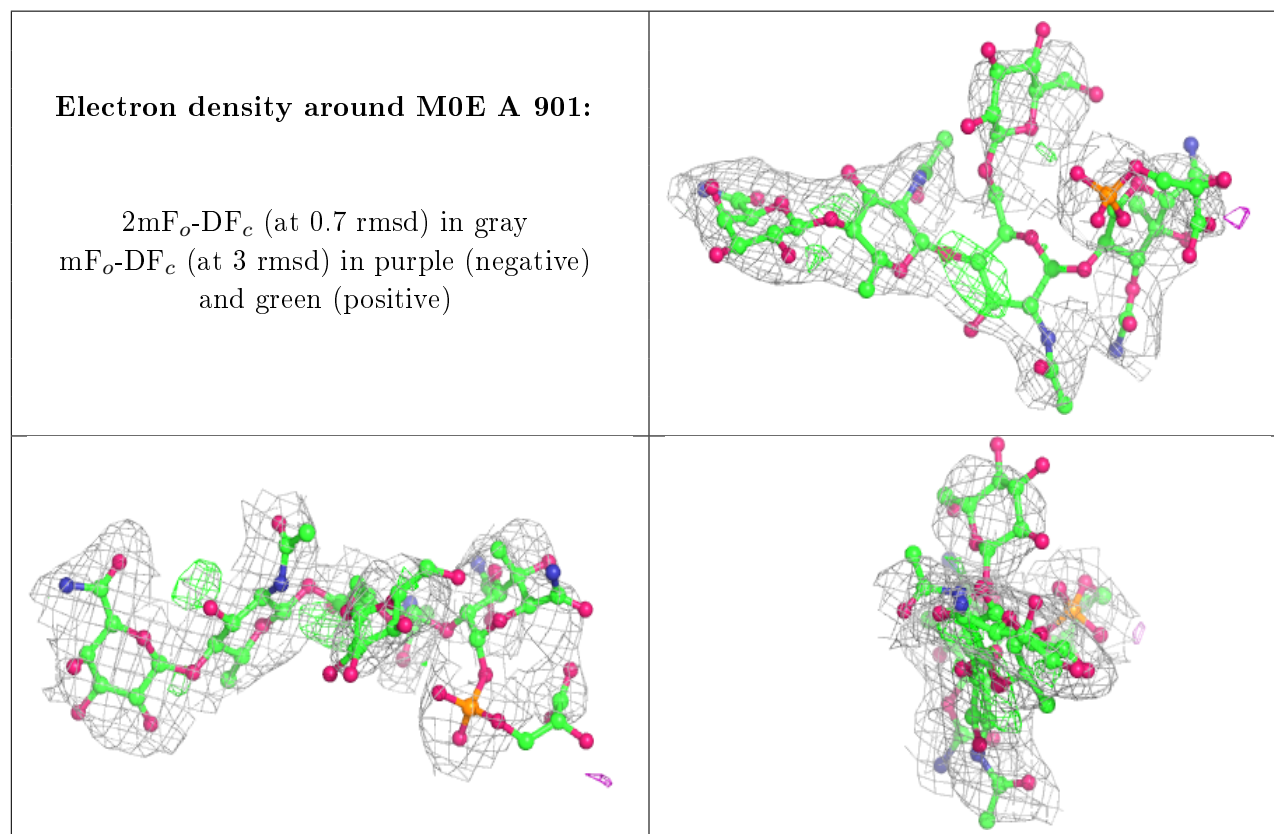
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	M0E	A	901	77/109	0.91	0.14	87,121,171,181	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.